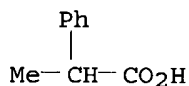


=> s e3  
L4 1 "2-PHENYLPROPIONIC ACID"/CN

=> d

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 492-37-5 REGISTRY  
CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Hydratropic acid (6CI, 7CI, 8CI)  
OTHER NAMES:  
CN (+)- $\alpha$ -Methylphenylacetic acid  
CN (+)-2-Phenylpropanoic acid  
CN (+)-2-Phenylpropionic acid  
CN (+)-Hydratropic acid  
CN (RS)-2-Phenylpropanoic acid  
CN (RS)-2-Phenylpropionic acid  
CN  $\alpha$ -Methylbenzeneacetic acid  
CN  $\alpha$ -Methylphenylacetic acid  
CN  $\alpha$ -Phenylpropionic acid  
CN 2-Phenylpropanoic acid  
CN **2-Phenylpropionic acid**  
CN DL-2-Phenylpropionic acid  
CN dl-PPA  
CN NSC 245033  
CN NSC 42872  
FS 3D CONCORD  
DR 2328-24-7  
MF C9 H10 O2  
CI COM  
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX,  
CHEMLIST, CSChem, DDFU, DRUGU, EMBASE, HODOC\*, IFICDB, IFIPAT, IFIUDB,  
IPA, MEDLINE, MSDS-OHS, NIOSHTIC, SPECINFO, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)  
Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*  
(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

708 REFERENCES IN FILE CA (1907 TO DATE)  
26 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
708 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
43 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file Hcaplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
20.94	23.51

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 10:41:11 ON 21 MAR 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Mar 2004 VOL 140 ISS 13  
FILE LAST UPDATED: 19 Mar 2004 (20040319/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 492-37-5/prep
      708 492-37-5
      3124510 PREP/RL
L5      223 492-37-5/PREP
          (492-37-5 (L) PREP/RL)

=> s 492-37-5/proc
      708 492-37-5
      3463782 PROC/RL
L6      89 492-37-5/PROC
          (492-37-5 (L) PROC/RL)

=> s 15 or 16
L7      312 L5 OR L6

=> s aryl alcohol or phenyl alcohol or phenyl halide
      186713 ARYL
      211016 ALCOHOL
          63 ARYL ALCOHOL
              (ARYL(W)ALCOHOL)
      310157 PHENYL
      211016 ALCOHOL
          20 PHENYL ALCOHOL
              (PHENYL(W)ALCOHOL)
      310157 PHENYL
      143837 HALIDE
          84 PHENYL HALIDE
              (PHENYL(W)HALIDE)
L8      167 ARYL ALCOHOL OR PHENYL ALCOHOL OR PHENYL HALIDE

=> s 17 and 18
L9      0 L7 AND L8

=> s aryl alcohol or phenyl alcohol or phenyl halide or olefin
      186713 ARYL
      211016 ALCOHOL
          63 ARYL ALCOHOL
              (ARYL(W)ALCOHOL)
      310157 PHENYL
      211016 ALCOHOL
          20 PHENYL ALCOHOL
              (PHENYL(W)ALCOHOL)
      310157 PHENYL
      143837 HALIDE
          84 PHENYL HALIDE
              (PHENYL(W)HALIDE)
      90365 OLEFIN
L10     90532 ARYL ALCOHOL OR PHENYL ALCOHOL OR PHENYL HALIDE OR OLEFIN

=> s 17 and 19
L11     0 L7 AND L9

=> s alcohol or halide or olefin
      211016 ALCOHOL
      143837 HALIDE
      90365 OLEFIN
```

L12 \* 437678 ALCOHOL OR HALIDE OR OLEFIN

=> s l12 and l7

L13 39 L12 AND L7

=> s l13 and palladium

138500 PALLADIUM

L14 13 L13 AND PALLADIUM

=> s l14 and py<2000

19722357 PY<2000

L15 10 L14 AND PY<2000

=> d 1-10 ibib abs hitstr

L15 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:606682 HCAPLUS

DOCUMENT NUMBER: 131:336794

TITLE: Highly efficient catalyst system for the synthesis of 2-arylpropionic acids by carbonylation

AUTHOR(S): Seayad, A.; Jayasree, S.; Chaudhari, R. V.

CORPORATE SOURCE: Homogeneous Catalysis Division, National Chemical Laboratory, Pune, 411008, India

SOURCE: Catalysis Letters (1999), 61(1,2), 99-103

CODEN: CALEER; ISSN: 1011-372X

PUBLISHER: Baltzer Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:336794

AB Carbonylation of 1-(4-isobutylphenyl)ethanol has been studied using a homogeneous catalyst system consisting of PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>/TsOH/LiCl. Higher reaction rates with TOF up to 1200 h<sup>-1</sup> and ibuprofen selectivity >95% have been achieved at 388 K under a CO partial pressure of 5.4 MPa. The reaction proceeds through the formation of 4-isobutylstyrene and 1-(4-isobutylphenyl)ethyl chloride as intermediates. The same catalyst system is shown to be effective for carbonylation of various α-arylethanol, vinyl aroms. and corresponding chloro derivs.

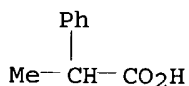
IT 492-37-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(catalytic carbonylation of (isobutylphenyl)ethanol and related compds.)

RN 492-37-5 HCAPLUS

CN Benzeneacetic acid, α-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:15905 HCAPLUS

DOCUMENT NUMBER: 130:124742

TITLE: Regioselective effect of CoCl<sub>2</sub> in olefin

hydrocarboxylation catalyzed by PdCl<sub>2</sub>(Ph<sub>3</sub>P)<sub>2</sub> complex

AUTHOR(S): Kron, T. E.; Terekhova, M. I.; Noskov, Yu. G.; Petrov, E. S.

CORPORATE SOURCE: Nauchno-Issled. Fiz.-Khim. Inst. im. L.Ya. Karpova, Gos. Nauchn. Tsentr Ross. Fed., Moscow, Russia

SOURCE: Zhurnal Fizicheskoi Khimii (1998), 72(10), 1834-1838

CODEN: ZFKHA9; ISSN: 0044-4537

PUBLISHER: MAIK Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Various factors such as CO pressure, water concentration, excess ligand L (PPh<sub>3</sub>),

and the presence of  $\text{CoCl}_2$  were examined for their influence on the regioselectivity of  $\text{PdCl}_2\text{L}_2$ -catalyzed hydrocarboxylation of 1-heptene, where regioselectivity  $S = 100 + r_1/(r_1 + r_2)$  was defined in terms of the rates of accumulation of normal and branched isomers  $r_1$  and  $r_2$ , resp. The bimetallic catalyst system led to an increase in  $S$  (from e.g., 66% without Co 79% with); this was observed even more dramatically with styrene, where an inversion in was was observed (from 23% without to 57% with).  $\text{CoCl}_2$  itself did not catalyze the hydrocarboxylation reaction. The synergistic mechanism was discussed.

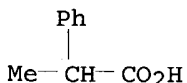
IT 492-37-5P, 2-Phenylpropanoic acid

RL: SPN (Synthetic preparation); PREP (Preparation)

(effect of  $\text{CoCl}_2$  and other reaction conditions on the regiochem. of olefin hydrocarboxylation catalyzed by  $\text{PdCl}_2(\text{Ph}_3\text{P})_2$  complex)

RN 492-37-5 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)



L15 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:600725 HCAPLUS

DOCUMENT NUMBER: 129:316015

TITLE: Biphasic Synthesis of 2-Phenylpropionic Acid and Ester by Interfacial Carbonylation of  $\alpha$ -Methylbenzyl Bromide

AUTHOR(S): Norman, Carnley; Wilhite, Benjamin A.; Pham, Duc; Lim, Phooi K.; Brown, Philip A.

CORPORATE SOURCE: Department of Chemical Engineering, North Carolina State University, Raleigh, NC, 27695-7905, USA

SOURCE: Organic Process Research & Development (1998), 2(6), 366-378

CODEN: OPRDFK; ISSN: 1083-6160

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An interfacial synthesis technique was successfully extended to the carbonylation of  $\alpha$ -methylbenzyl bromide in an organic-aqueous sodium hydroxide mixture at 35-60 °C and 1 atm using surface-active palladium-(4-dimethylaminophenyl)diphenylphosphine complex as the catalyst and dodecyl sodium sulfate as the emulsifier. Depending on the reaction conditions, 2-phenylpropionate in the form of sodium salt and an ester was obtained in 0-83% yield, along with varying amts. of side products that included  $\alpha$ -methylbenzyl alc., 2,3-diphenylbutane, di( $\alpha$ -methylbenzyl)ether, and an asym. ether derived from the substrate and an alc. medium. When 2-methyl-1-butanol or 2-ethyl-1-hexanol was used as the organic phase, 2-phenylpropionate ester and sodium salt were obtained in 40-83% yield, with a maximum yield obtained at an optimal aqueous base concentration of about 5 M. At a lower aqueous base concentration,

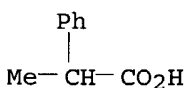
more of  $\alpha$ -methylbenzyl alc. was formed, whereas at a higher aqueous base concentration, more of 2,3-diphenylbutane and asym. ether were formed. When toluene was used as the organic phase, 2-phenylpropionate salt was obtained in less than 13% yield, and the major side product was  $\alpha$ -methylbenzyl alc. at a low aqueous base concentration and 2,3-diphenylbutane at a high aqueous base concentration. In all cases, the formation of 2,3-diphenylbutane was accompanied by a stoichiometric formation of carbonate. The latter implicates the involvement of an oxidative intermediate-tentatively identified as hypobromous acid-that could deactivate the catalyst complex through ligand degradation. Along with the carbonylation reaction, carbon monoxide also underwent a slow, base-induced hydrolysis reaction to form formic acid. With 2-ethyl-1-hexanol as the organic phase, the carbonylation of  $\alpha$ -methylbenzyl bromide showed an apparent temperature-dependent activation energy, a first-order dependence each on the substrate, catalyst, and ligand concns. up to the catalyst concentration of 0.0020 M and a ligand:catalyst

\* ratio of 3:1, and a variable-order dependence on the carbon monoxide pressure that switched from first to zero order as the carbon monoxide pressure was increased above 450 mmHg. A reaction mechanism is proposed which yields model rate and yield expressions in accord with the exptl. findings. Results of control expts. with  $\alpha,\alpha$ -dibromotoluene in a toluene-aqueous sodium hydroxide mixture indicate that replacement of the  $\alpha$ -Me group in  $\alpha$ -methylbenzyl bromide by a second bromo group suppressed the formation of substituted benzyl alc. and coupled product. They suggest that the broad product distribution in the carbonylation of  $\alpha$ -methylbenzyl bromide relative to the carbonylation of benzyl chloride and  $\alpha,\alpha$ -dibromotoluene is attributable to the electron-releasing  $\alpha$ -Me group making the substrate susceptible to hydrolysis and coupling reactions.

IT 492-37-5P, 2-Phenylpropionic acid  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (biphasic preparation of phenylpropionate via interfacial carbonylation of methylbenzyl bromide)

RN 492-37-5 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:594127 HCAPLUS

DOCUMENT NUMBER: 127:277806

TITLE: Catalytic conversions in water. Part 6. A novel biphasic hydrocarboxylation of olefins catalyzed by **palladium** TPPTS complexes (TPPTS=P(C<sub>6</sub>H<sub>4</sub>-m-SO<sub>3</sub>Na)<sub>3</sub>)

AUTHOR(S): Papadogianakis, Georgios; Verspui, Goran; Maat, Leendert; Sheldon, Roger A.

CORPORATE SOURCE: Laboratory of Organic Chemistry and Catalysis, Delft University of Technology, Delft, 2628 BL, Neth.

SOURCE: Catalysis Letters (1997), 47(1), 43-46

CODEN: CALEER; ISSN: 1011-372X

PUBLISHER: Baltzer

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:277806

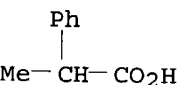
AB Exceptionally high catalytic activities (TOF> 2500h<sup>-1</sup>) have been achieved in the biphasic hydrocarboxylation of propene catalyzed by water-soluble Pd/TPPTS complexes. The activity was even higher than that exhibited by organic-soluble Pd/PPh<sub>3</sub> systems. This contrasts with the general perception that biphasic catalysis normally exhibits lower rates compared to analogous reactions in organic media. The hydrocarboxylation of 4-isobutylstyrene to ibuprofen and of styrene in a two-phase system is also reported.

IT 492-37-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (biphasic hydrocarboxylation of olefins catalyzed by **palladium** TPPTS complexes)

RN 492-37-5 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1996:469962 HCAPLUS  
 DOCUMENT NUMBER: 125:142279  
 TITLE: Preparation of arylacetic and arylpropionic acids  
 INVENTOR(S): Sheldon, Roger A.; Maat, Leendert; Papadogianakis, Georgios  
 PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA  
 SOURCE: U.S., 6 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5536874	A	19960716	US 1994-347027	19941130 <--
WO 9626177	A1	19960829	WO 1995-US14578	19951109 <--

W: ES, GB, JP

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRIORITY APPLN. INFO.: US 1994-347027 19941130

OTHER SOURCE(S): CASREACT 125:142279; MARPAT 125:142279

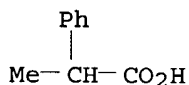
AB The title compds. R1C(R2)(R3)COOR4 [I; R1 = halo, OH, C1-8 alkyl, etc.; R2, R3 = H, halo, Ph, etc.; R4 = H, C1-8 alkyl, Ph, etc.] were prepared by carbonylation of (substituted) arylcarbinols R1C(R2)(R3)OH in a two-phase system wherein one phase is an aqueous medium which contains (1) a catalyst which is a water-soluble complex consisting essentially of a Group VIII metal and a hydrophilic ligand such as **palladium** complexed with trisulfonated triphenylphosphine, and (2) optionally an acid, and the second phase comprises said arylcarbinol. Thus, carbonylation of 4-fluorobenzyl alc. in the presence of Pd(OAc)<sub>2</sub> and Na salt of trisulfonated triphenylphosphine in H<sub>2</sub>O/PhMe afforded I [R1 = 4-FC<sub>6</sub>H<sub>4</sub>; R2 = R3 = R4 = H].

IT 492-37-5P, 2-Phenylpropionic acid

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**  
 (Preparation)

(preparation of arylacetic and arylpropionic acids)

RN 492-37-5 HCAPLUS

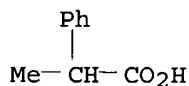
CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)

ACCESSION NUMBER: 1995:340126 HCAPLUS  
 DOCUMENT NUMBER: 122:314239  
 TITLE: Carbonylation of styrene and other olefins to keto compounds with cationic **palladium** complexes  
 AUTHOR(S): Pisano, Carmelina; Consiglio, Giambattista  
 CORPORATE SOURCE: Swiss Federal Institute of Technology, Department of Industrial Engineering Chemistry, Zurich, CH-8092, Switz.  
 SOURCE: Gazzetta Chimica Italiana (1994), 124(10), 393-401  
 CODEN: GCITA9; ISSN: 0016-5603  
 PUBLISHER: Societa Chimica Italiana  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

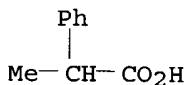
AB Various carbonylation reactions, i.e., the synthesis of aldehydes (hydroformylation), of ketones and of alternating copolymers by reaction of olefins with carbon monoxide can be catalyzed by **palladium** complexes of the type PdX<sub>2</sub>L<sub>2</sub> (where L<sub>2</sub> = mono- or bidentate phosphorus or nitrogen ligand, X = anion with low coordination ability). The chemoselectivity of the catalytic systems is influenced both by the ligand

and by the anion. Analogous nickel complexes are not active for carbonylation under similar reaction conditions whereas platinum complexes catalyze only hydroformylation. Using styrene as the substrate, conditions were found that produce either (E)-1,5-diphenylpent-1-en-3-one or (E)-1,4-diphenylpent-1-en-3-one with high selectivity even in the presence of hydrogen. Furthermore, the influence of various reaction parameters on the activity and on the selectivity for this carbonylation reaction has been investigated. With o-methylstyrene the formation of ketones is less selective than for styrene under the same reaction conditions. With other aromatic substrates such as 2-phenylpropene or (E)-1-phenylpropene only aldehyde formation was achieved. By contrast aliphatic substrates give oligomeric ketones.

IT 492-37-5P, 2-Phenylpropionic acid  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (carbonylation of alkenes to carbonyl compds. with cationic  
**palladium** complexes)  
 RN 492-37-5 HCAPLUS  
 CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)

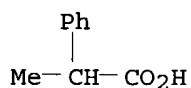


L15 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1993:448918 HCAPLUS  
 DOCUMENT NUMBER: 119:48918  
 TITLE: Regiochemical synthesis of straight chain acids by the  
**palladium(II)** catalyzed hydrocarboxylation of  
 olefins with oxalic acid  
 AUTHOR(S): El Ali, Bassam; Alper, Howard  
 CORPORATE SOURCE: Ottawa-Carleton Chem. Inst., Univ. Ottawa, ON, K1N  
 6N5, Can.  
 SOURCE: Journal of Molecular Catalysis (1993),  
 80(3), 377-81  
 CODEN: JMCADS; ISSN: 0304-5102  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 119:48918  
 AB Olefins react with carbon monoxide and oxalic acid, catalyzed by  
**palladium** acetate in the presence of 1,4-  
 bis(diphenylphosphino)butane, to give linear carboxylic acids  
 regioselectively. Thus, styrene afforded PhCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H and PhCHMeCO<sub>2</sub>H in a  
 ratio of 85:15 (86% yield). This process shows excellent functional group  
 tolerance.  
 IT 492-37-5P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (preparation of)  
 RN 492-37-5 HCAPLUS  
 CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)



L15 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1993:101236 HCAPLUS  
 DOCUMENT NUMBER: 118:101236  
 TITLE: Formic acid-**palladium** acetate-1,4-  
 bis(diphenylphosphino)butane: an effective catalytic  
 system for regioselective hydrocarboxylation of simple  
 and functionalized olefins  
 AUTHOR(S): El Ali, Bassam; Alper, Howard  
 CORPORATE SOURCE: Ottawa-Carleton Chem., Univ. Ottawa, Ottawa, ON, K1N

6N5, Can.  
 SOURCE: Journal of Molecular Catalysis (1992),  
 77(1), 7-13  
 CODEN: JMCADS; ISSN: 0304-5102  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 118:101236  
 AB Reaction of mono- and disubstituted olefins, e.g., PhCH:CH<sub>2</sub>, with formic acid, catalytic quantities of **palladium** acetate and 1,4-bis(diphenylphosphino)butane, in a carbon monoxide atmosphere, affords carboxylic acids, e.g., PhCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, in 45-98% yield. The reaction is regioselective and, in a number of cases, regiospecific for the straight-chain acid. Functional groups such as trimethylsilyl, aldehyde, ketone, nitrile, acid and amide and trisubstituted olefins can be tolerated in this reaction.  
 IT 492-37-5P  
 RL: SPN (Synthetic preparation); **PREP** (Preparation)  
 (preparation of)  
 RN 492-37-5 HCAPLUS  
 CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)



L15 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1990:440159 HCAPLUS  
 DOCUMENT NUMBER: 113:40159  
 TITLE: Carbonylation of arylalkyl halides in preparation of  $\alpha$ -arylpropionic acids as antiinflammatories  
 INVENTOR(S): Elango, Varadaraj  
 PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA  
 SOURCE: Eur. Pat. Appl., 12 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 338852	A1	19891025	EP 1989-303995	19890421 <--
EP 338852	B1	19941130		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 1338592	A1	19960910	CA 1989-596739	19890414 <--
JP 01311044	A2	19891215	JP 1989-100365	19890421 <--
ES 2065373	T3	19950216	ES 1989-303995	19890421 <--
US 6555704	B1	20030429	US 1995-445593	19950522
PRIORITY APPLN. INFO.:				
			US 1988-185184	A 19880422
			US 1990-537865	B1 19900614
			US 1992-834979	B1 19920214
			US 1992-973542	B1 19921109

OTHER SOURCE(S): MARPAT 113:40159  
 AB ArchMeCO<sub>2</sub>H [Ar = Ph, polynuclear aromatic, optionally substituted by (cyclo)alkyl, alkoxy, phenoxy, halo, oxo], useful as analgesics, antipyretics, and inflammation inhibitors such as ibuprofen, were prepared by carbonylation of ArchCHClMe (I) with CO in a protic acidic aqueous medium containing H<sup>+</sup> and dissociated **halide** ions, in the presence of a Pd complex, e.g., PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub> as a catalyst, at 10-225° and 100-5000 psig, with the molar ratio of dissociated ions to I of 0.1-5, preferably 0.2-2.0. I were obtained by haloalkylation of the parent aromatic compds. with a hydrogen **halide** and an alkylation agent, e.g., MeCHO, (MeO)<sub>2</sub>CHMe, etc., in the presence of a Lewis acid. A mixture of MeCHO and Me<sub>2</sub>CHCH<sub>2</sub>Ph (II) was added dropwise to a mixture of II and ZnCl<sub>2</sub> at ≤10° over 2 h, HCl was passed through the whole at room temperature during .apprx.2 h, and the stirring continued for 6 h to give I [Ar



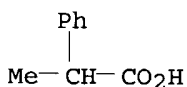
~ = 4-(Me2CHCH2)C6H4] (III). The latter in C6H6 containing PhCOMe was heated 4 h at 110° in the presence of PdCl2(PPh3)2, concentrated HCl, and KHSO4, in an autoclave pressurized with 800 psig CO, to give 72% ibuprofen based on a 99% conversion of III.

IT 492-37-5P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(preparation of, by carbonylation of arylethyl halides)

RN 492-37-5 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)



L15 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:405876 HCAPLUS

DOCUMENT NUMBER: 97:5876

TITLE: Selective phase transfer and **palladium**  
(0)-catalyzed carbonylation, carbalkoxylation, and  
reduction reactions

AUTHOR(S): Alper, Howard; Hashem, Khaled; Heveling, Josef

CORPORATE SOURCE: Dep. Chem., Univ. Ottawa, Ottawa, ON, K1N 9B4, Can.

SOURCE: Organometallics (1982), 1(6), 775-8

CODEN: ORGND7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (Ph3P)4Pd catalyzes the carbonylation of benzylic halides to carboxylic acids using 5 N NaOH and CH2Cl2 at room temperature and 1 atmospheric. Although the presence of (C6H13)4N+ HSO4- (a phase-transfer catalyst) improves the yield, a quaternary ammonium salt is not necessary in these reactions. Reduction (and coupling) of halides occurs using [(PhCH:CH)2CO]2Pd as the catalyst under phase-transfer conditions (no reaction takes place in the absence of the phase-transfer catalyst). Esters were obtained by the phase-transfer-catalyzed carbonylation of halides in the presence of (Ph2PCH2CH2PPh2)2Pd, while acids were the principal products in the absence of the quaternary ammonium salt.

IT 492-37-5P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(preparation of)

RN 492-37-5 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)

